Electronic Structure of MgO: O K X-ray Fluorescence Measurements

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MgO with its sodium chloride structure is regarded as a prototype for a simple oxide and has thus been object of many theoretical and experimental studies dealing with the electronic structure. The bulk electronic structure has been studied with several methods like ARUPS [1] and electron excited XES [2]. A good understanding of theproperties is required because, from a technological point of view, MgO is an important material with many applications as catalyst.

A new method to investigate the electronic structure is RIXS (Resonant Inelastic X-ray Scattering) and highly resolved spectra can be recorded at the ALS Beamline 8.0. First measurements were carried out on HOPG, a material with a well known electronic band structure. It was shown that the observed spectra can give some momentum resolved information about the valence band dispersion [3]. Because RIXS doesn't remove electrons from the system, no charging effects occour like in photoelectron spectroscopy.

We measured the O Kα emission spectra in MgO excited with photon energies between 530 and 550 eV. Also absorption spectra have been measured in the range from 527 to 562 eV. Data interpretation has been done based on first-principle calculations of electronic structure by the all-electron full potential linearized augmented plane wave method (FLAPW). FLAPW calculations have been done with the WIEN97 implementation of the code [4].

The solid line in Fig. 1. displays the absoprtion spectra at the O 1s threshold. The 1s $\rightarrow$ 2p absorption starts to contribute at an excitation energy of about 530 eV with a maximum at 535 eV. This all over maximum is followed by a sholder at about 539 eV. Two more absorption maxima can be found at 546 and 556.5 eV excitation energy. The

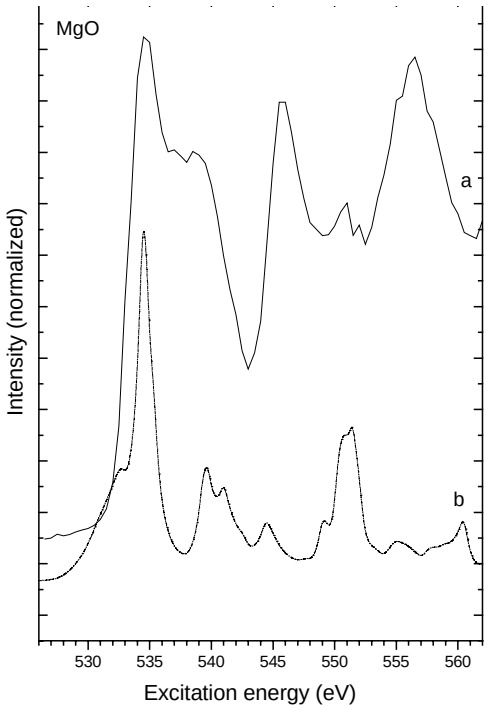

Fig 1: Experimental (a) and theoretical absoprtion spectra (b) at the O Kα edge.

absorption spectra probe the density of empty states in the valence band formed by O 2p states. This partial density of states (pDOS) is illustrated by the calculated OKα absorption spectra. Between E_{exc}=526eV and E_{exc}= 543 eV the calculation fits to the measurement very well. Above E_{exc}= 543 eV the maxima in the calculation are at the same photon energy compared to the measurement, but the intensities don't describe the measurement sufficiently.

The theoretical absorption spectrum is deduced from the calculated band structure shown in Fig. 2. In this picture the diameter of the circles represent the pDOS of the oxygen 2p states in the valence and conduction bands.

In soft X-ray emission, when the excitation energy goes through the threshold at E_{exc}=533 eV the conduction band is reached only at the Γ-point of the Brillouin-zone. With increasing the excitation energy, only empty states are reached in the Δ- and Λ direction.
If the following de-excitation occours in resonance with the excitation process, the emission originates from the same points in the Brillouin zone [3]. In the case of MgO, first one peak should be observable. It should split into two peaks with distances growing with increasing excitation energy.

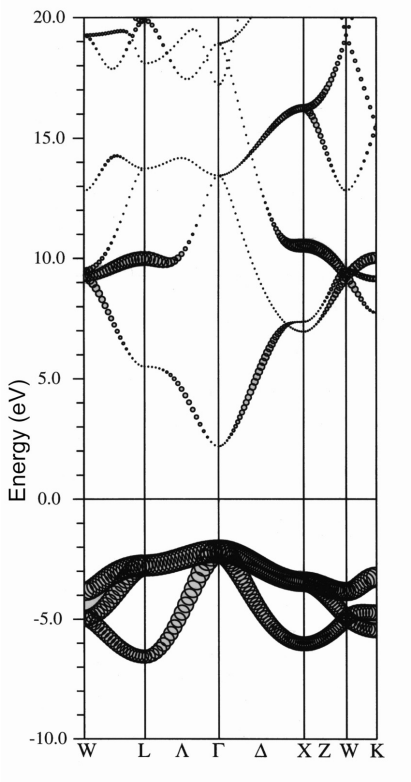

Fig 2: Calculated O 2p band structure based on FLAPW method [4].

Fig. 3 displays emission spectra recorded at excitation energies from 528.5 eV to 535.5 eV and 548.5 eV. Considering the band structure in Fig. 2 these energies were just suitable to excite electrons from the O 1s level to the lowest conduction band in ΓXW- direction. The spectra show a main peak at 525.1 eV and a second peak at 521.8 eV. Accordingly the difference in emission energy is 3.3 eV. This is in agreement with the band structure calculation as well as with electron excited XES measurements [2]. The spectra reflect the O2p density of states in the valence band. No shift in emission energy can be observed due to the variation of excitation energy. Also the ratio in intensity of the two peaks doesn't change. This leads to the

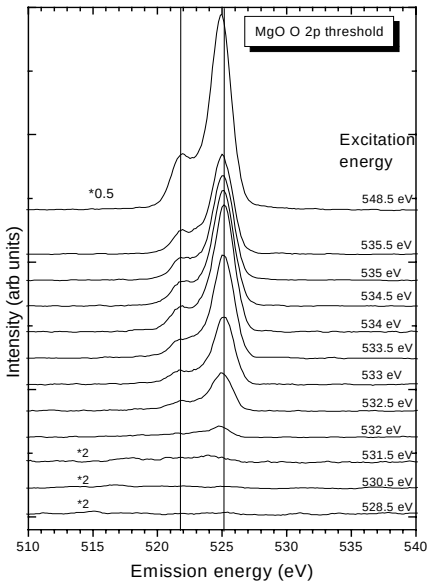

Fig 3: O Kα emission spectra in dependance on the excitation energy.

conclusion that no resonant processes occour at the O Kα threshold in MgO. Only normal X-ray emission can be obtained, the de-excitation process happens independantly of the excitation process.

References

1. L. H. Tjeng, A. R. Vos and G. A. Sawatzky, Surf. Sci, 235, 269 (1990)
2. P. Jonnard, F. Vergand, C. Bonnelle, Phys. Rev. B 57, no 19, 12 111 (1998)
3. J.A. Carlisle, E.L. Shirley, E.A. Hudson, L.J. Terminello, T.A. Callcott, J.J. Jia, D.L. Ederer, R.C.C. Perera, and F.J. Himpsel, Phys. Rev. Lett. 74, 1234 (1995)
4. P. Blaha, K. Schwarz, J. Luitz, WIEN97, Vienna Universtiy of Technology 1997. Improved and updated Unix version of the original copyrighted WIEN-code, which was published by P. Blaha, K. Schwartz, P. Soratin, S.B. Trickey, Comput. Phys. Commun. 59, 399 (1990)

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